

Test of Information Theory on the Boltzmann Equation

Kim Hyeon-Deuk *

*Graduate School of Human and Environmental Studies,
Kyoto University, Kyoto 606-8501, Japan*

Hisao Hayakawa[†]

*Department of Physics, Yoshida-South Campus,
Kyoto University, Kyoto 606-8501, Japan*

Abstract

We examine information theory using the steady-state Boltzmann equation. In a nonequilibrium steady-state system under steady heat conduction, the thermodynamic quantities from information theory are calculated and compared with those from the steady-state Boltzmann equation. We have found that information theory is inconsistent with the steady-state Boltzmann equation.

PACS numbers: 05.20.-y, 05.20.Dd, 51.10.+y, 51.30.+i

* kim@yuragi.jinkan.kyoto-u.ac.jp

† hisao@yuragi.jinkan.kyoto-u.ac.jp

I. INTRODUCTION

The behaviors of gases in nonequilibrium states have received considerable attention from the standpoint of understanding the characteristics of nonequilibrium phenomena. The Boltzmann equation is widely accepted as one of the most reliable models for describing gases in nonequilibrium phenomena, so that various attempts have been conducted on solving the Boltzmann equation.[1, 2, 3, 4, 5, 6, 7] Recently, we have derived the explicit velocity distribution function of the steady-state Boltzmann equation for hard-core molecules to second order in density and temperature gradients by the Chapman-Enskog method.[8]

On the other hand, in the early 1960s, Zubarev[9, 10] has developed nonequilibrium statistical mechanics and obtained the general form of a nonequilibrium velocity distribution function with the aid of the maximum entropy principle. Thereafter the nonequilibrium velocity distribution function to first order has been derived by expanding the Zubarev form for the nonequilibrium velocity distribution function under some constraints.[11]

Jou and his coworkers have derived the nonequilibrium velocity distribution function to second order by expanding the Zubarev form for the nonequilibrium velocity distribution function to second order under the some constraints, which is called information theory.[12, 13, 14, 15, 16, 17] Information theory has attracted interest in the development of a general framework for nonlinear nonequilibrium statistical mechanics. There is even a text book on information theory.[12] Jou *et al.* have applied the velocity distribution function from information theory to nonequilibrium dilute gases.[12, 13, 14, 15, 16, 17, 18, 19] There are also several applications of information theory to other microscopic theories, such as radiation[20, 21, 22, 23, 24], nonviscous gases[25, 26] and chemically reacting gases[27]. Nettleton claimed that information theory provides a statistical mechanical basis of irreversible processes and of extended thermodynamics which is consistent with the laws of thermodynamics.[28] He has developed the maximum entropy formalism and applied it to a dilute gas system.[29, 30, 31, 32, 33] However, in the actual applications, it is not easy to examine the validity of information theory. In order to demonstrate the invalidity of information theory, it is necessary to find qualitative differences between information theory and the microscopic theories in the applications. In fact, though we have recently compared the effect of heat flux on the rate of chemical reaction calculated from information theory with those which we have calculated from kinetic theories, we have found no qualitative

differences among them.[34] We find no reports which conclude that information theory is not an appropriate theory to describe nonequilibrium phenomena.

However, as was mentioned in refs. 13 and 19, more examinations of information theory should be carried out from the microscopic viewpoint to confirm whether there exists universality in nonlinear nonequilibrium statistical mechanics. In the present paper, we check the validity of information theory from a kinetic view point: we examine whether information theory coincides with the steady-state Boltzmann equation, at least qualitatively, in a nonequilibrium steady state.

Suppose a dilute gas system subject to a temperature gradient along the x -axis in a steady state whose velocity distribution function is expressed as $f = f(x, \mathbf{v})$. We introduce five conserved quantities and a heat flux playing important roles in both information theory and the steady-state Boltzmann equation. We define the density:

$$n(x) \equiv \int f d\mathbf{v}, \quad (1)$$

and the temperature:

$$\frac{3n(x)\kappa T(x)}{2} \equiv \int \frac{m\mathbf{v}^2}{2} f d\mathbf{v}, \quad (2)$$

with m the mass of a molecule and κ the Boltzmann constant. We assume no mean flow:

$$\int m\mathbf{v} f d\mathbf{v} = \mathbf{0}, \quad (3)$$

where $\mathbf{0}$ denotes the zero vector. Furthermore, we define the heat flux:

$$J_x \equiv \int \frac{m\mathbf{v}^2}{2} v_x f d\mathbf{v}. \quad (4)$$

It should be emphasized that the heat flux J_x calculated from eq.(4) must be uniform in a steady state. Actually, in the case for the steady-state Boltzmann equation, its solubility conditions lead to the heat flux J_x being constant to second order.[8]

The organization of this paper is as follows. We will introduce information theory in § II. In § III, we will introduce the velocity distribution functions of the steady-state Boltzmann equation for both hard-core and Maxwell molecules to second order by the Chapman-Enskog method. In § IV, we will apply the velocity distribution functions to a nonequilibrium steady-state system under steady heat conduction, and compare the results of thermodynamic quantities from information theory with those from the steady-state Boltzmann equation. Our discussion and conclusion are written in § V.

II. INFORMATION THEORY

Let us introduce information theory proposed by Jou *et al.*[12, 13, 14, 15, 16, 17]. The Zubarev form for the nonequilibrium velocity distribution function under a heat flux can be obtained by maximizing the nonequilibrium entropy, defined as

$$S(x) \equiv -\kappa \int f \log f d\mathbf{v}, \quad (5)$$

under the constraints of the density (1), the temperature (2), no mean flow (3) and the heat flux (4) which is now *assumed* to be uniform as well as $n\kappa T$ by contrast with the case for the steady-state Boltzmann equation.[8] Jou *et al.* have finally obtained the nonequilibrium velocity distribution function to second order in the heat flux J_x by expanding the Zubarev's nonequilibrium velocity distribution function to second order as

$$f = \frac{1}{Z} \exp\left(-\beta \frac{m\mathbf{v}^2}{2}\right) \left[1 - \frac{4J_x}{5n\kappa T} \left(\frac{m}{2\kappa T}\right)^{\frac{1}{2}} c_x \left(\frac{5}{2\beta\kappa T} - \mathbf{c}^2\right) + \frac{4mJ_x^2}{25n^2\kappa^3T^3} c_x^2 \left(\frac{5}{2\beta\kappa T} - \mathbf{c}^2\right)^2\right], \quad (6)$$

with the scaled velocity $\mathbf{c} \equiv (m/2\kappa T)^{1/2}\mathbf{v}$. Here Z is given by

$$Z = \frac{1}{n} \left(\frac{2\pi}{\beta m}\right)^{\frac{3}{2}} \left(1 + \frac{mJ_x^2}{5n^2\kappa^3T^3}\right), \quad (7)$$

in order to normalize f . The parameter β is found to be

$$\beta = \frac{1}{\kappa T} \left(1 + \frac{2mJ_x^2}{5n^2\kappa^3T^3}\right) \equiv \frac{1}{\kappa\theta}, \quad (8)$$

and has been used by Jou *et al.* to introduce θ as a nonequilibrium temperature. From eq.(8) it is clear that the nonequilibrium temperature θ is not identical with the temperature T defined in eq.(2), and θ is lower than T . [12, 13, 14, 15, 16, 17, 18, 22, 23]

By expanding the velocity distribution function (6) to second order in J_x , we obtain the expression for the *modified* velocity distribution function:

$$f = f^{(0)} \left\{1 - \frac{3J_x}{2n\kappa T} \left(\frac{\pi m}{2\kappa T}\right)^{\frac{1}{2}} c_x S_{\frac{3}{2}}^1(\mathbf{c}^2) + \frac{2mJ_x^2}{5n^2\kappa^3T^3} (1 - \mathbf{c}^2) + \frac{mJ_x^2}{5n^2\kappa^3T^3} c_x^2 [3\sqrt{\pi} S_{\frac{1}{2}}^2(\mathbf{c}^2) + 2]\right\}, \quad (9)$$

with the local Maxwellian distribution function $f^{(0)} = n(m/2\pi\kappa T)^{3/2} \exp(-\mathbf{c}^2)$. Here n and T have been identified in eqs.(1) and (2). This *modified* velocity distribution function has

been also obtained and used by Fort and Cukrowski[18]. Note that $S_k^p(X)$ is the Sonine polynomial. (see, *e.g.* ref. 8) We have confirmed that the *modified* velocity distribution function still satisfies constraints (3) and (4), while the corrections appearing in eqs.(7) and (8) no longer appear in the density (1) and the temperature (2) with the *modified* velocity distribution function expressed in eq.(9). We adopt this *modified* velocity distribution function instead of the velocity distribution function shown in eq.(6) to calculate macroscopic quantities in this paper. This adoption is based on the fact that the corrections in eqs.(7) and (8) are not significant, although Jou *et al.*[12, 13, 14, 15, 16, 17, 18] believe that the correction appearing in eq.(8) has important physical meaning. (see also § V)

III. KINETIC THEORY: THE STEADY-STATE BOLTZMANN EQUATION

We introduce the velocity distribution function of the steady-state Boltzmann equation for hard-core molecules which we have derived in ref. 8 valid to second order in density and the temperature gradient. In a nonequilibrium steady-state system under the temperature gradient along x -axis, it can be written as

$$\begin{aligned} f = f^{(0)} \{ & 1 - \frac{4J_x}{5b_{11}n\kappa T} \left(\frac{m}{2\kappa T}\right)^{\frac{1}{2}} \sum_{r \geq 1} r! b_{1r} c_x \Gamma(r + \frac{5}{2}) S_{\frac{3}{2}}^r(\mathbf{c}^2) \\ & + \frac{4096mJ_x^2}{5625b_{11}^2n^2\kappa^3T^3} \left[\sum_{r \geq 2} r! b_{0r} \Gamma(r + \frac{3}{2}) S_{\frac{1}{2}}^r(\mathbf{c}^2) \right. \\ & \left. + \sum_{r \geq 0} r! b_{2r} (2c_x^2 - c_y^2 - c_z^2) \Gamma(r + \frac{7}{2}) S_{\frac{5}{2}}^r(\mathbf{c}^2) \right] \}, \end{aligned} \quad (10)$$

where the specific values for b_{1r} , b_{0r} and b_{2r} are found in Table I. Note that we show only the values for 7th Sonine approximation.[8]

For our calculation of the macroscopic quantities, we also adopt the precise velocity distribution function of the steady-state Boltzmann equation for Maxwell molecules to second order derived by Schamberg[35]. It becomes

$$\begin{aligned} f = f^{(0)} \{ & 1 - \frac{4J_x}{5n\kappa T} \left(\frac{m}{2\kappa T}\right)^{\frac{1}{2}} c_x \Gamma(\frac{7}{2}) S_{\frac{3}{2}}^1(\mathbf{c}^2) + \frac{4096mJ_x^2}{5625n^2\kappa^3T^3} \left[\sum_{r=2,3} r! b_{0r} \Gamma(r + \frac{3}{2}) S_{\frac{1}{2}}^r(\mathbf{c}^2) \right. \\ & \left. + \sum_{r=1,2} r! b_{2r} (2c_x^2 - c_y^2 - c_z^2) \Gamma(r + \frac{7}{2}) S_{\frac{5}{2}}^r(\mathbf{c}^2) \right] \}, \end{aligned} \quad (11)$$

where the precise values for b_{0r} and b_{2r} are written in Table II. It should be mentioned that the first-order velocity distribution function in eq.(11) is identical with that for information

theory shown in eq.(9), while the second-order velocity distribution functions are different from each other.

IV. TEST OF INFORMATION THEORY

Now the velocity distribution functions to second order given in eqs.(9), (10) and (11) shall be applied to the nonequilibrium steady-state system. Note that all the definitions of physical quantities in this paper are the same as those in ref. 8.

To begin with, the pressure tensor in the nonequilibrium steady state P_{ij} becomes

$$P_{ij} = n\kappa T \left(\delta_{ij} + \lambda_P^{ij} \frac{mJ_x^2}{n^2\kappa^3T^3} \right), \quad (12)$$

with the unit tensor δ_{ij} and the numerical tensor components λ_P^{ij} shown in Table III. Note that the off-diagonal components of λ_P^{ij} are zero and that $\lambda_P^{yy} = \lambda_P^{zz}$ is satisfied. We have found that λ_P^{ij} for information theory is qualitatively different from those for the steady-state Boltzmann equation for both hard-core and Maxwell molecules: P_{xx} becomes larger than P_{yy} and P_{zz} for information theory[14, 15], while P_{xx} becomes smaller than P_{yy} and P_{zz} for the steady-state Boltzmann equation for hard-core molecules, and no second-order corrections appear in P_{ij} for the steady-state Boltzmann equation for Maxwell molecules.

Each component of the kinetic temperature in the nonequilibrium steady state, i.e. T_i for $i = x, y$ and z is also calculated as

$$\frac{n\kappa T_i}{2} = \frac{n\kappa T}{2} \left(1 + \lambda_{T_i} \frac{mJ_x^2}{n^2\kappa^3T^3} \right), \quad (13)$$

for $i = x, y$ and z . Numerical values for the constants λ_{T_i} for $i = x, y$ and z are given in Table III. Note that $\lambda_{T_y} = \lambda_{T_z}$. We find that λ_{T_i} for information theory is qualitatively different from those for the steady-state Boltzmann equation for both hard-core and Maxwell molecules: T_x becomes larger than T_y and T_z for information theory, while T_x becomes smaller than T_y and T_z for the steady-state Boltzmann equation for hard-core molecules, and no corrections appear in T_i for the steady-state Boltzmann equation for Maxwell molecules.

The Shannon entropy in the nonequilibrium steady state becomes

$$S(x) = -n\kappa \log \left[n \left(\frac{m}{2\pi\kappa T} \right)^{\frac{3}{2}} \right] + \frac{3}{2}n\kappa + \lambda_S \frac{mJ_x^2}{n\kappa^2T^3}, \quad (14)$$

to second order with the numerical constant λ_S written in Table III. It is found that λ_S for information theory is identical to that obtained from the steady-state Boltzmann equation

for Maxwell molecules, while it is slightly different from λ_S calculated from the steady-state Boltzmann equation for hard-core molecules. This is because the correction term for the Shannon entropy is determined only by the first-order velocity distribution function, as was indicated in ref. 12.

V. DISCUSSION AND CONCLUSION

It is seen that the first-order velocity distribution functions for the steady-state Boltzmann equation for both hard-core and Maxwell molecules, i.e. the first-order terms in eqs.(10) and (11), are consistent with that derived by expanding Zubarev's velocity distribution function[9, 10, 11]. This consistency is attributed to the fact that a nonequilibrium correction in the nonequilibrium entropy should appear to even order of a nonequilibrium flux, *e.g.* $\delta S \propto -J_x^2$, in order that the nonequilibrium entropy has a maximum at $J_x = 0$, and that a thermodynamic force $F = \partial \delta S / \partial J_x$ which drives a nonequilibrium system towards the state of equilibrium is proportional to the nonequilibrium flux.[36] This fact leads to a conclusion that the nonequilibrium entropy is not modified from the local equilibrium entropy to first order, and that the Shannon-type entropy is appropriate as the nonequilibrium entropy to first order.

On the other hand, we have confirmed that both forms (10) and (11) of the second-order velocity distribution functions differ from that suggested by information theory[12, 13, 14, 15, 16, 17]. Although Jou *et al.* have applied information theory to nonequilibrium dilute gases[12, 13, 14, 15, 16, 17, 18, 19], we have found that information theory contradicts the steady-state Boltzmann equation: all the macroscopic quantities for information theory except for the Shannon entropy S in eq.(14) are qualitatively different from those for the steady-state Boltzmann equation for both hard-core and Maxwell molecules. These qualitative differences between information theory and the steady-state Boltzmann equation still appear no matter which boundary condition is adopted. It is conjectured that the entropy defined in eq.(5) is not appropriate as the nonequilibrium entropy to second order, though the Shannon-type entropy has been widely used as the nonequilibrium entropy to any order.[9, 10, 11, 12, 13, 28, 29, 30, 31, 32, 33, 36] We emphasize that it is probably the first time to find qualitative differences between information theory and nonequilibrium microscopic theories and demonstrate that information theory is inconsistent with the nonequi-

librium microscopic theories. We can conclude that, though quite a few statistical physicists have believed the existence of a universal velocity distribution function in the nonequilibrium steady state by maximizing the Shannon-type entropy[9, 10, 11, 12, 13, 28, 29, 30, 31, 32, 33], the universal velocity distribution function does not exist in the nonequilibrium steady state. It is also worth mentioning that, although information theory based on the Tsallis entropy has been also developed[37, 38], the general form of the velocity distribution function for information theory based on the Tsallis entropy[37, 38] cannot be expanded even to first order because the expanded velocity distribution function diverges.

We have also confirmed that, in all the macroscopic quantities calculated in the present paper, there are no differences between the results from the *modified* velocity distribution function given in eq.(9) and those from Jou's velocity distribution function shown in eq.(6) so long as the same boundary condition is adopted. This suggests that the nonequilibrium temperature θ has no physical significance. We emphasize that the identifications of the density, the temperature and the mean flow (see eqs.(11), (12) and (13) in ref. 8) do not affect the physical properties of the velocity distribution function for the steady-state Boltzmann equation[8], and that those identifications must be satisfied for the conservation laws in the case for the steady-state Bhatnagar-Gross-Krook(BGK) equation.[39, 40]

Acknowledgments

We would like to express our sincere thanks to H. Tasaki who made us aware of the significance of understanding nonequilibrium steady-state phenomena. This research was essentially inspired by him. We are grateful to S. Sasa who has always had crucial, interesting and cheerful discussions with us and has encouraged us to carry out these calculations. The authors also appreciate Ooshida T., A. Yoshimori, M. Sano, J. Wakou, K. Sato, H. Kuninaka, T. Mizuguti, T. Chawanya, S. Takesue and H. Tomita for fruitful discussions and useful comments. This study has been supported partially by the Hosokawa Powder Technology Foundation, the Inamori Foundation and Grant-in-Aid for Scientific Research (No. 13308021).

-
- [1] S. Chapman and T. G. Cowling: *The Mathematical Theory of Non-uniform Gases*(Cambridge University Press, London, 1990).
 - [2] J. A. McLennan: *Introduction to Nonequilibrium Statistical Mechanics*(Prentice Hall, Englewood Cliffs, New Jersey, 1990). This book can be obtained from <http://www.lehigh.edu/~ljm3/ljm3.html>
 - [3] P. Résibois and M. De Leener: *Classical Kinetic Theory of Fluids*(A Wiley-Interscience Publication, New York, 1977).
 - [4] M. N. Kogan: *Rarefied Gas Dynamics*(Plenum Press, New York, 1969).
 - [5] S. Flügge: *Thermodynamics of Gases*(Springer-Verlag, Berlin, 1958).
 - [6] J. H. Ferziger and H. G. Kaper: *Mathematical Theory of Transport Processes in Gases*(North-Holland Publishing Company, Amsterdam and London, 1972).
 - [7] C. Cercignani: *Mathematical Methods in Kinetic Theory*(Plenum Press, New York and London, 1990).
 - [8] Kim H.-D. and H. Hayakawa: J. Phys. Soc. Jpn. **72** (2003) 1904.
 - [9] D. Zubarev, V. Morozov and G. Ropke: *Statistical Mechanics of Nonequilibrium Processes I, II* (Akademie Verlag, Berlin, 1996).
 - [10] D. Zubarev: Dokl. Akad. Nauk SSSR, Ser. Fiz. **140** (1961) 92.
 - [11] A. Katz: *Principles of Statistical Mechanics* (Freeman, San Francisco, 1967).
 - [12] D. Jou, J. Casas-Vázquez and G. Lebon: *Extended Irreversible Thermodynamics* (Springer, Berlin, 2001).
 - [13] D. Jou, J. Casas-Vázquez and G. Lebon: J. Non-Equilib. Thermodyn. **23** (1998) 277.
 - [14] J. Camacho and D. Jou: Phys. Rev. E **52** (1995) 3490.
 - [15] R. Dominguez and D. Jou: Phys. Rev. E **51** (1995) 158.
 - [16] J. Casas-Vázquez and D. Jou: Phys. Rev. E **49** (1994) 1040.
 - [17] D. Jou and M. Criado-Sancho: Physica A **292** (2001) 75.
 - [18] J. Fort and A. S. Cukrowski: Acta Phys. Polo. B **29** (1998) 1633.
 - [19] J. Fort and A. S. Cukrowski: Chem. Phys. **222** (1997) 59.
 - [20] R. Dominguez-Cascante and J. Faraudo: Phys. Rev. E **54** (1996) 6933.
 - [21] J. Fort: Phys. Rev. E **59** (1999) 3710.

- [22] J. Fort, D. Jou and J. E. Llebot: Physica A **248** (1998) 97.
- [23] J. Fort, D. Jou and J. E. Llebot: Physica A **269** (1999) 439.
- [24] J. Fort and J. E. Llebot: J. Math. Phys. **39** (1998) 345.
- [25] M. S. Mongiovi: Phys. Rev. E **63** (2001) 061202.
- [26] M. S. Mongiovi: Math. Comp. Model. **36** (2002) 951.
- [27] J. Fort, J. Casas-Vázquez and V. Méndez: J. Phys. Chem. B **103** (1999) 860.
- [28] R. E. Nettleton: J. Chem. Phys. **106** (1997) 10311.
- [29] R. E. Nettleton: Phys. Rev. E **54** (1996) 2147.
- [30] R. E. Nettleton: Phys. Rev. E **53** (1996) 1241.
- [31] R. E. Nettleton: J. Phys. Chem. **100** (1996) 11005.
- [32] R. E. Nettleton: Z. Phys. Chem. **196** (1996) 177.
- [33] B. C. Eu: J. Chem. Phys. **108** (1998) 5834.
- [34] Kim H.-D. and H. Hayakawa: Chem. Phys. Lett. **372** (2003) 314.
- [35] R. Schamberg: Ph. D thesis, California Institute of Technology (1947).
- [36] M. B. Romero and R. M. Velasco: Physica A **222** (1995) 161.
- [37] A. R. Plastino, M. Casas and A. Plastino: Physica A **280** (2000) 289.
- [38] Q. A. Wang, Chaos, Solitons and Fractals, **12** (2001) 1431.
- [39] A. Santos, J. J. Brey, C. S. Kim and J. W. Dufty: Phys. Rev. A **39** (1989) 320.
- [40] C. S. Kim, J. W. Dufty, A. Santos and J. J. Brey: Phys. Rev. A **39** (1989) 328.

TABLE I: Numerical constants b_{1r} , b_{0r} and b_{2r} in eq.(10). All the values are ones for 7th Sonine approximation.

	b_{1r}	b_{0r}	b_{2r}
0	0	1	-3.320×10^{-2}
1	1.025	0	-1.276×10^{-1}
2	4.892×10^{-2}	4.380×10^{-1}	6.414×10^{-2}
3	3.715×10^{-3}	-5.429×10^{-2}	5.521×10^{-3}
4	2.922×10^{-4}	-4.098×10^{-3}	4.214×10^{-4}
5	2.187×10^{-5}	-3.184×10^{-4}	3.106×10^{-5}
6	1.492×10^{-6}	-2.087×10^{-5}	1.861×10^{-6}
7	8.322×10^{-8}	—	—

TABLE II: Numerical constants b_{0r} and b_{2r} in eq.(11).

	b_{0r}	b_{2r}
1	—	$\frac{75}{896}$
2	$\frac{825}{1024}$	$\frac{125}{1536}$
3	$-\frac{25}{256}$	—

TABLE III: The numerical constants for the macroscopic quantities: the precise values for information theory, the 7th Sonine approximation values for hard-core molecules and the exact values for Maxwell molecules.

	λ_P^{xx}	λ_P^{yy}	λ_{T_x}	λ_{T_y}	λ_S
information theory	$\frac{12}{25}$	$-\frac{6}{25}$	$\frac{6}{25}$	$-\frac{3}{25}$	$-\frac{1}{5}$
hard-core molecules	-4.600×10^{-2}	2.300×10^{-2}	-2.300×10^{-2}	1.150×10^{-2}	-2.035×10^{-1}
Maxwell molecules	0	0	0	0	$-\frac{1}{5}$